



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:07 PM UTC

PDB ID : 8R70 / pdb_00008r70
Title : Polysaccharide lyase BtPL33HA (BT4410) Y291A with HA dp4
Authors : Cartmell, A.
Deposited on : 2023-11-23
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

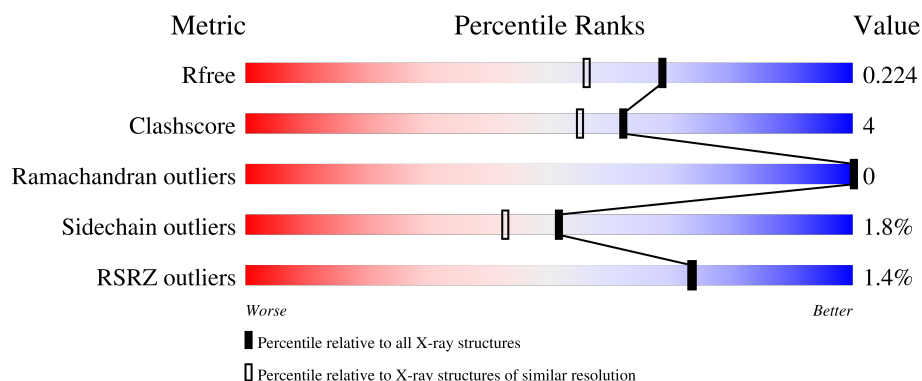
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	644	0% 85% 10% .
1	B	644	2% 82% 11% 6%
2	C	3	100%
3	D	4	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MES	A	702	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20540 atoms, of which 9811 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Heparinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	618	Total	C	H	N	O	S	123	3	0
			9900	3178	4901	855	932	34			
1	B	608	Total	C	H	N	O	S	120	2	0
			9703	3117	4802	835	915	34			

There are 54 discrepancies between the modelled and reference sequences:

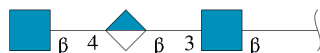
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q89ZG7
A	2	GLY	-	expression tag	UNP Q89ZG7
A	3	SER	-	expression tag	UNP Q89ZG7
A	4	SER	-	expression tag	UNP Q89ZG7
A	5	HIS	-	expression tag	UNP Q89ZG7
A	6	HIS	-	expression tag	UNP Q89ZG7
A	7	HIS	-	expression tag	UNP Q89ZG7
A	8	HIS	-	expression tag	UNP Q89ZG7
A	9	HIS	-	expression tag	UNP Q89ZG7
A	10	HIS	-	expression tag	UNP Q89ZG7
A	11	SER	-	expression tag	UNP Q89ZG7
A	12	SER	-	expression tag	UNP Q89ZG7
A	13	GLY	-	expression tag	UNP Q89ZG7
A	14	LEU	-	expression tag	UNP Q89ZG7
A	15	VAL	-	expression tag	UNP Q89ZG7
A	16	PRO	-	expression tag	UNP Q89ZG7
A	17	ARG	-	expression tag	UNP Q89ZG7
A	18	GLY	-	expression tag	UNP Q89ZG7
A	19	SER	-	expression tag	UNP Q89ZG7
A	20	HIS	-	expression tag	UNP Q89ZG7
A	21	MET	-	expression tag	UNP Q89ZG7
A	22	ALA	-	expression tag	UNP Q89ZG7
A	23	SER	-	expression tag	UNP Q89ZG7
A	24	ASN	-	expression tag	UNP Q89ZG7
A	25	ALA	-	expression tag	UNP Q89ZG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	TYR	-	expression tag	UNP Q89ZG7
A	291	ALA	TYR	engineered mutation	UNP Q89ZG7
B	1	MET	-	initiating methionine	UNP Q89ZG7
B	2	GLY	-	expression tag	UNP Q89ZG7
B	3	SER	-	expression tag	UNP Q89ZG7
B	4	SER	-	expression tag	UNP Q89ZG7
B	5	HIS	-	expression tag	UNP Q89ZG7
B	6	HIS	-	expression tag	UNP Q89ZG7
B	7	HIS	-	expression tag	UNP Q89ZG7
B	8	HIS	-	expression tag	UNP Q89ZG7
B	9	HIS	-	expression tag	UNP Q89ZG7
B	10	HIS	-	expression tag	UNP Q89ZG7
B	11	SER	-	expression tag	UNP Q89ZG7
B	12	SER	-	expression tag	UNP Q89ZG7
B	13	GLY	-	expression tag	UNP Q89ZG7
B	14	LEU	-	expression tag	UNP Q89ZG7
B	15	VAL	-	expression tag	UNP Q89ZG7
B	16	PRO	-	expression tag	UNP Q89ZG7
B	17	ARG	-	expression tag	UNP Q89ZG7
B	18	GLY	-	expression tag	UNP Q89ZG7
B	19	SER	-	expression tag	UNP Q89ZG7
B	20	HIS	-	expression tag	UNP Q89ZG7
B	21	MET	-	expression tag	UNP Q89ZG7
B	22	ALA	-	expression tag	UNP Q89ZG7
B	23	SER	-	expression tag	UNP Q89ZG7
B	24	ASN	-	expression tag	UNP Q89ZG7
B	25	ALA	-	expression tag	UNP Q89ZG7
B	26	TYR	-	expression tag	UNP Q89ZG7
B	291	ALA	TYR	engineered mutation	UNP Q89ZG7

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	H	N	O	6	0	0
			71	22	30	2	17			

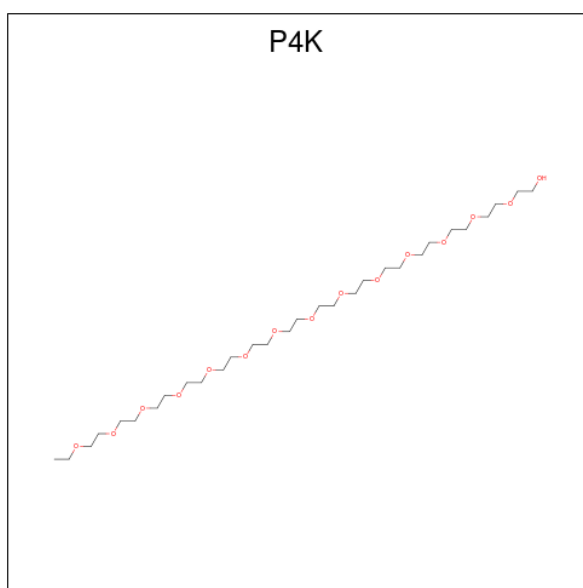
- Molecule 3 is an oligosaccharide called beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-d

eoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



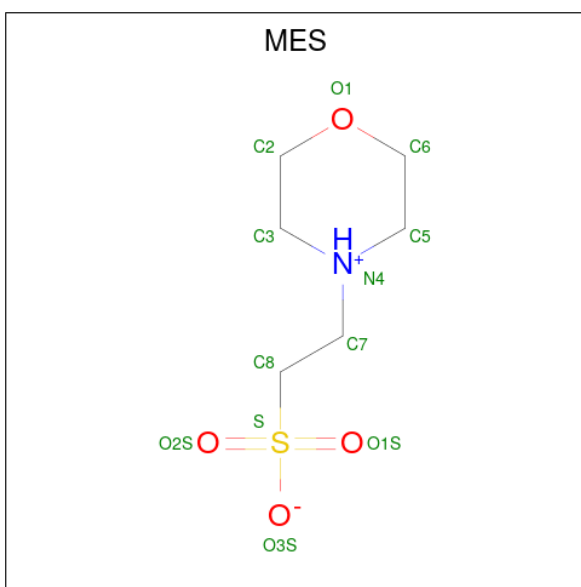
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	H	N	O	8	0	0
			90	28	37	2	23			

- Molecule 4 is polyethylene glycol (CCD ID: P4K) (formula: $C_{30}H_{62}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	1	0
			28	8	16	4		
4	B	1	Total	C	H	O	1	0
			21	6	12	3		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn		
			1	1	0	0
6	B	1	Total	Zn		
			1	1	0	0

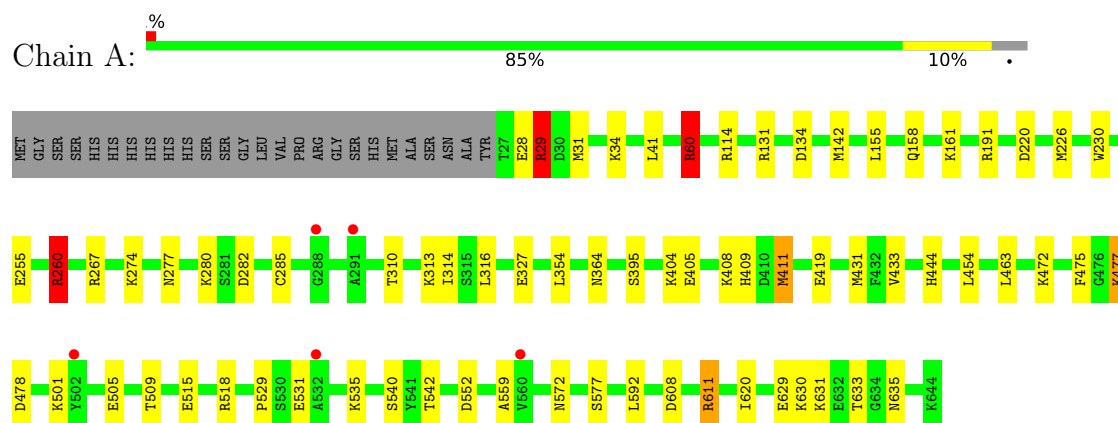
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	434	Total	O		
			434	434	0	0
7	B	266	Total	O		
			266	266	0	0

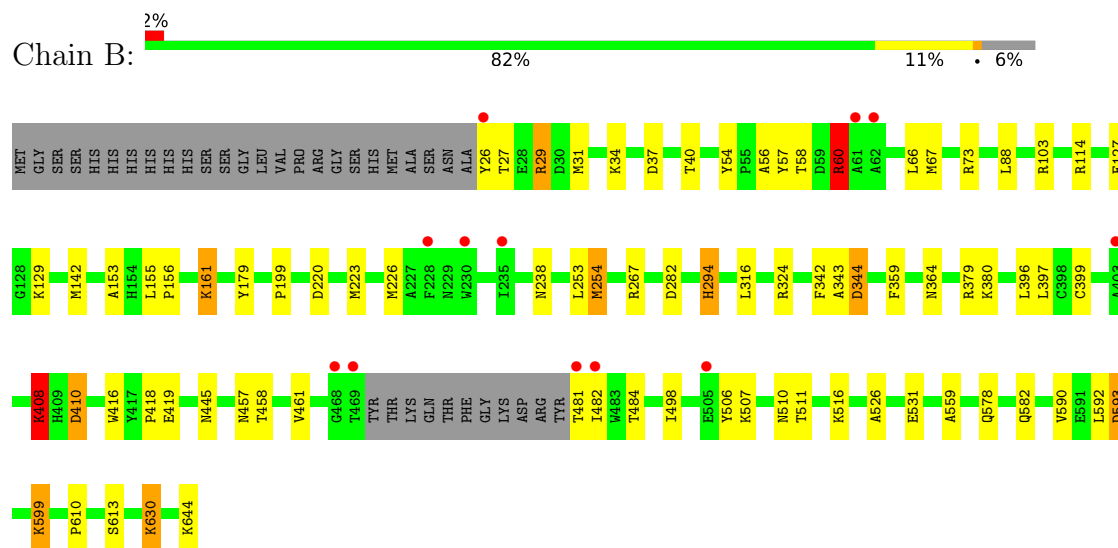
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Heparinase



• Molecule 1: Heparinase



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

100%

MAG1
BDF2
MAG3
BDF4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.64Å 137.30Å 202.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.70 – 1.80 113.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	87.0 (113.70-1.80) 92.0 (113.70-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.181 , 0.223 0.183 , 0.224	Depositor DCC
R_{free} test set	7185 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20540	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, MES, P4K, BDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.92	2/5120 (0.0%)	1.34	28/6927 (0.4%)
1	B	0.80	0/5019	1.36	25/6792 (0.4%)
All	All	0.86	2/10139 (0.0%)	1.35	53/13719 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	6
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	ARG	NE-CZ	6.23	1.40	1.33
1	A	611	ARG	NE-CZ	5.19	1.38	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	THR	CA-CB-OG1	-11.29	92.66	109.60
1	B	254	MET	CG-SD-CE	9.54	121.89	100.90
1	A	60	ARG	CD-NE-CZ	9.49	137.69	124.40
1	A	260	ARG	CD-NE-CZ	8.39	136.15	124.40
1	A	419	GLU	CB-CG-CD	-8.16	98.73	112.60
1	B	630	LYS	N-CA-CB	-8.08	98.29	110.90
1	A	409	HIS	CA-CB-CG	-7.88	105.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	ASP	CA-CB-CG	7.55	120.15	112.60
1	B	359	PHE	CA-CB-CG	7.51	121.31	113.80
1	B	294	HIS	CA-CB-CG	-7.50	106.30	113.80
1	A	608	ASP	CB-CA-C	-7.45	96.36	110.67
1	A	60	ARG	NE-CZ-NH1	7.15	128.65	121.50
1	A	411	MET	CG-SD-CE	-6.94	85.64	100.90
1	B	380	LYS	CB-CA-C	6.82	119.28	109.26
1	B	578	GLN	CB-CA-C	6.65	120.53	109.89
1	B	324	ARG	CD-NE-CZ	6.43	133.40	124.40
1	A	611	ARG	NE-CZ-NH2	6.42	124.97	119.20
1	A	313	LYS	CB-CA-C	6.36	122.89	110.67
1	A	477	LYS	O-C-N	-6.33	115.58	122.79
1	A	29	ARG	CG-CD-NE	-6.29	98.16	112.00
1	A	134	ASP	CA-CB-CG	6.25	118.85	112.60
1	B	511	THR	CA-CB-OG1	-6.21	100.29	109.60
1	A	226	MET	CG-SD-CE	-6.15	87.36	100.90
1	B	179	TYR	CA-C-N	6.08	126.69	119.94
1	B	179	TYR	C-N-CA	6.08	126.69	119.94
1	A	60	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	B	408	LYS	CG-CD-CE	5.75	124.53	111.30
1	A	220	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	282	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	58	THR	CA-CB-OG1	-5.69	101.07	109.60
1	B	484	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	629	GLU	CB-CG-CD	-5.67	102.97	112.60
1	A	515	GLU	CB-CG-CD	5.62	122.15	112.60
1	B	60	ARG	CB-CG-CD	5.56	124.09	111.30
1	B	324	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	B	410	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	542	THR	CA-CB-OG1	-5.48	101.37	109.60
1	A	611	ARG	CG-CD-NE	5.47	124.03	112.00
1	B	344	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	54	TYR	N-CA-C	-5.34	103.45	110.39
1	A	313	LYS	CB-CG-CD	5.32	123.53	111.30
1	B	220	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	199	PRO	N-CA-C	5.29	120.81	113.98
1	A	531	GLU	CB-CA-C	-5.26	100.25	110.46
1	B	593	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	516	LYS	N-CA-CB	-5.24	102.47	110.33
1	A	191	ARG	CD-NE-CZ	-5.13	117.22	124.40
1	A	131	ARG	CD-NE-CZ	5.11	131.55	124.40
1	A	475	PHE	CB-CA-C	5.08	118.14	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	ASN	CA-CB-CG	-5.08	107.52	112.60
1	A	191	ARG	CA-CB-CG	-5.08	103.94	114.10
1	A	535	LYS	N-CA-CB	5.06	118.03	110.14
1	A	629	GLU	CB-CA-C	-5.03	100.40	110.42

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ARG	Sidechain
1	A	260	ARG	Sidechain
1	A	267[A]	ARG	Sidechain
1	A	29	ARG	Sidechain
1	A	518	ARG	Sidechain
1	A	60	ARG	Sidechain
1	A	611	ARG	Sidechain
1	B	114	ARG	Sidechain
1	B	267	ARG	Sidechain
1	B	29	ARG	Sidechain
1	B	445	ASN	Peptide
1	B	481	THR	Peptide
1	B	60	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4999	4901	4889	44	1
1	B	4901	4802	4790	39	1
2	C	41	30	33	0	0
3	D	53	37	40	0	0
4	A	12	16	0	1	0
4	B	9	12	0	0	0
5	A	12	13	13	11	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	434	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	266	0	0	11	0
All	All	10729	9811	9765	82	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:ASP:HB3	7:B:1042:HOH:O	1.41	1.20
1:B:419:GLU:HG3	7:B:829:HOH:O	1.48	1.11
1:A:572:ASN:HB3	7:A:1088:HOH:O	1.48	1.10
1:A:327:GLU:OE1	4:A:701:P4K:O9	1.74	1.03
1:A:277:ASN:HD22	5:A:702:MES:H72	1.45	0.82
1:A:31:MET:HE3	1:A:316:LEU:HD13	1.63	0.80
1:A:274:LYS:CD	5:A:702:MES:H82	2.13	0.79
1:B:31:MET:HE3	1:B:316:LEU:HD13	1.66	0.76
1:B:254:MET:HE1	7:B:935:HOH:O	1.88	0.73
1:A:230:TRP:CH2	5:A:702:MES:H21	2.25	0.71
1:A:31:MET:CE	1:A:316:LEU:HD13	2.22	0.68
1:B:254:MET:CE	7:B:935:HOH:O	2.40	0.68
1:A:405[B]:GLU:OE2	7:A:801:HOH:O	2.12	0.67
1:B:582:GLN:NE2	7:B:801:HOH:O	2.26	0.66
1:A:364:ASN:HB3	7:A:816:HOH:O	1.95	0.66
1:B:379:ARG:HB2	1:B:379:ARG:NH1	2.11	0.66
1:A:477:LYS:O	7:A:802:HOH:O	2.14	0.66
1:A:60:ARG:HD3	7:A:1121:HOH:O	1.96	0.65
1:A:477:LYS:O	1:A:478:ASP:HB2	1.97	0.65
1:A:572:ASN:HB3	7:A:1177:HOH:O	1.97	0.65
1:A:274:LYS:HD2	5:A:702:MES:H82	1.79	0.64
1:A:274:LYS:HD3	5:A:702:MES:H82	1.80	0.62
1:A:364:ASN:CB	7:A:816:HOH:O	2.48	0.62
1:A:444:HIS:NE2	7:A:806:HOH:O	2.31	0.61
1:A:477:LYS:O	1:A:478:ASP:CB	2.47	0.59
1:A:29:ARG:O	1:A:34:LYS:HE2	2.02	0.59
1:A:285:CYS:SG	7:A:1153:HOH:O	2.57	0.58
1:B:26:TYR:N	7:B:804:HOH:O	2.37	0.58
1:B:498:ILE:HD13	1:B:531:GLU:HG2	1.85	0.58
1:B:408:LYS:HD2	1:B:410:ASP:CG	2.28	0.58
1:B:238:ASN:HB2	1:B:294:HIS:O	2.05	0.57
1:B:593:ASP:CB	7:B:1042:HOH:O	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:LEU:HB3	1:B:254:MET:HE2	1.87	0.55
1:A:509:THR:HG23	7:A:879:HOH:O	2.06	0.54
1:A:277:ASN:HD22	5:A:702:MES:C7	2.21	0.52
1:B:559:ALA:HB1	1:B:630:LYS:HG2	1.90	0.52
1:A:277:ASN:CB	5:A:702:MES:H32	2.40	0.52
1:B:127:GLU:HG2	1:B:129:LYS:HG3	1.92	0.52
1:B:253:LEU:HB3	1:B:254:MET:CE	2.40	0.51
1:A:552:ASP:O	1:A:635:ASN:HB2	2.11	0.51
1:B:379:ARG:HB2	1:B:379:ARG:HH11	1.75	0.50
1:A:559:ALA:HB1	1:A:630:LYS:HG2	1.94	0.49
1:A:404:LYS:NZ	7:A:804:HOH:O	2.25	0.49
1:B:37:ASP:HB2	7:B:847:HOH:O	2.13	0.49
1:A:501:LYS:HD2	1:A:529:PRO:HB3	1.96	0.48
1:B:592:LEU:HD23	1:B:592:LEU:C	2.39	0.47
1:A:631:LYS:HE3	1:A:633:THR:O	2.15	0.47
1:B:29:ARG:O	1:B:34:LYS:HE2	2.15	0.47
1:B:408:LYS:HD2	1:B:410:ASP:OD2	2.14	0.47
1:A:255:GLU:OE1	1:A:260:ARG:NH1	2.49	0.46
1:A:155:LEU:O	1:A:158:GLN:HG2	2.16	0.45
1:B:610:PRO:HA	1:B:613:SER:OG	2.16	0.45
1:B:457:ASN:C	1:B:458:THR:HG23	2.41	0.45
1:B:103:ARG:HG2	1:B:153:ALA:HB2	1.99	0.45
1:A:310:THR:HG21	1:A:314:ILE:HD12	1.98	0.45
1:A:354:LEU:HD23	1:A:395:SER:HB2	1.98	0.45
1:B:66:LEU:HD11	1:B:397:LEU:HA	1.99	0.44
1:B:416:TRP:O	1:B:418:PRO:HD3	2.17	0.44
1:B:254:MET:HE2	7:B:935:HOH:O	2.14	0.44
1:B:342:PHE:O	1:B:343:ALA:HB3	2.18	0.44
1:B:644:LYS:NZ	7:B:821:HOH:O	2.51	0.44
1:A:161:LYS:HG2	7:A:1134:HOH:O	2.17	0.43
1:B:67:MET:HE2	1:B:396:LEU:HD13	1.99	0.43
1:A:433:VAL:HG22	1:A:454:LEU:HD13	1.99	0.43
1:A:592:LEU:C	1:A:592:LEU:HD23	2.43	0.43
1:B:419:GLU:CG	7:B:829:HOH:O	2.32	0.42
1:B:461:VAL:HG11	1:B:590:VAL:HG21	2.00	0.42
1:A:230:TRP:CZ3	5:A:702:MES:H21	2.55	0.42
1:B:156:PRO:O	1:B:161:LYS:HA	2.19	0.42
1:A:277:ASN:HB3	5:A:702:MES:H32	2.02	0.42
1:A:431:MET:HG3	7:A:1130:HOH:O	2.19	0.42
1:A:277:ASN:ND2	5:A:702:MES:H72	2.25	0.42
1:B:155:LEU:N	1:B:156:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:MET:HE3	1:B:226:MET:CE	2.50	0.41
1:A:463:LEU:C	1:A:463:LEU:HD12	2.46	0.41
1:B:56:ALA:O	1:B:57:TYR:C	2.63	0.41
1:A:620:ILE:HD13	1:A:620:ILE:HG21	1.80	0.41
1:A:142:MET:SD	1:A:142:MET:C	3.04	0.41
1:B:142:MET:C	1:B:142:MET:SD	3.04	0.41
1:A:277:ASN:HB2	5:A:702:MES:H32	2.02	0.41
1:A:142:MET:HG2	1:B:88:LEU:HD11	2.03	0.40
1:B:506:TYR:HA	1:B:526:ALA:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:SER:HG	1:B:599:LYS:HZ3[2_454]	1.27	0.33

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	619/644 (96%)	595 (96%)	24 (4%)	0	100	100
1	B	606/644 (94%)	579 (96%)	27 (4%)	0	100	100
All	All	1225/1288 (95%)	1174 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	533/551 (97%)	525 (98%)	8 (2%)	57	49
1	B	523/551 (95%)	512 (98%)	11 (2%)	47	36
All	All	1056/1102 (96%)	1037 (98%)	19 (2%)	51	43

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	41	LEU
1	A	280	LYS
1	A	408	LYS
1	A	411	MET
1	A	472	LYS
1	A	505	GLU
1	A	540	SER
1	B	27	THR
1	B	60	ARG
1	B	73	ARG
1	B	161	LYS
1	B	344	ASP
1	B	364	ASN
1	B	399	CYS
1	B	408	LYS
1	B	482	ILE
1	B	507	LYS
1	B	599	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	115	GLN
1	A	256	ASN
1	A	294	HIS
1	A	394	GLN
1	A	441	ASN
1	A	457	ASN
1	A	504	GLN

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Mol	Chain	Res	Type
1	A	510	ASN
1	A	588	GLN
1	A	642	GLN
1	B	231	GLN
1	B	457	ASN
1	B	486	GLN
1	B	588	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

7 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	2	15,15,15	1.86	3 (20%)	21,21,21	1.96	8 (38%)
2	BDP	C	2	2	12,12,13	1.76	4 (33%)	14,17,19	2.04	3 (21%)
2	NAG	C	3	2	14,14,15	3.01	9 (64%)	17,19,21	2.84	6 (35%)
3	NAG	D	1	3	15,15,15	1.36	3 (20%)	21,21,21	1.00	0
3	BDP	D	2	3	12,12,13	2.44	6 (50%)	14,17,19	2.02	5 (35%)
3	NAG	D	3	3	14,14,15	3.06	9 (64%)	17,19,21	2.81	9 (52%)
3	BDP	D	4	3	12,12,13	3.60	7 (58%)	14,17,19	2.99	9 (64%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2	-	2/6/26/26	0/1/1/1
2	BDP	C	2	2	-	0/4/21/24	0/1/1/1
2	NAG	C	3	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3	-	0/6/26/26	0/1/1/1
3	BDP	D	2	3	-	0/4/21/24	0/1/1/1
3	NAG	D	3	3	-	2/6/23/26	0/1/1/1
3	BDP	D	4	3	-	2/4/21/24	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	NAG	C8-C7	-7.54	1.34	1.50
2	C	3	NAG	C8-C7	-7.38	1.35	1.50
3	D	4	BDP	O5-C1	6.16	1.54	1.43
3	D	4	BDP	C5-C6	5.46	1.64	1.53
3	D	4	BDP	O6A-C6	5.41	1.38	1.22
2	C	1	NAG	C2-N2	5.34	1.54	1.45
3	D	4	BDP	O6B-C6	4.93	1.46	1.30
3	D	3	NAG	O7-C7	4.63	1.33	1.23
3	D	4	BDP	O5-C5	4.56	1.52	1.43
3	D	2	BDP	O3-C3	4.19	1.53	1.43
2	C	3	NAG	C1-C2	4.07	1.57	1.52
3	D	2	BDP	C4-C5	3.35	1.58	1.53
2	C	3	NAG	C4-C5	3.29	1.60	1.53
3	D	2	BDP	C4-C3	3.12	1.60	1.52
2	C	3	NAG	O5-C5	3.04	1.49	1.43
3	D	2	BDP	C1-C2	2.95	1.59	1.52
2	C	2	BDP	C4-C5	2.90	1.58	1.53
2	C	3	NAG	O7-C7	2.84	1.29	1.23
2	C	2	BDP	O6A-C6	2.81	1.30	1.22
3	D	1	NAG	C1-C2	2.81	1.56	1.52
2	C	1	NAG	O1-C1	2.75	1.48	1.39
2	C	2	BDP	C1-C2	2.69	1.58	1.52
2	C	3	NAG	C4-C3	2.67	1.59	1.52
3	D	3	NAG	C1-C2	2.66	1.56	1.52
3	D	3	NAG	O3-C3	2.64	1.49	1.43
3	D	2	BDP	C2-C3	2.60	1.56	1.52
3	D	3	NAG	O4-C4	2.59	1.49	1.43
3	D	3	NAG	C3-C2	2.55	1.57	1.52
3	D	2	BDP	O2-C2	2.51	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	BDP	O4-C4	2.40	1.48	1.43
2	C	3	NAG	O5-C1	2.23	1.47	1.43
3	D	3	NAG	C6-C5	2.23	1.59	1.51
2	C	3	NAG	C2-N2	2.23	1.50	1.46
3	D	3	NAG	C4-C3	2.20	1.58	1.52
3	D	1	NAG	C2-N2	2.18	1.49	1.45
2	C	3	NAG	O4-C4	2.09	1.48	1.43
3	D	1	NAG	C4-C3	2.09	1.57	1.52
3	D	3	NAG	C4-C5	2.08	1.57	1.53
2	C	1	NAG	O4-C4	-2.06	1.37	1.43
3	D	4	BDP	C4-C5	2.06	1.56	1.53
3	D	4	BDP	C4-C3	2.05	1.57	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	NAG	C8-C7-N2	7.62	128.75	116.12
2	C	3	NAG	O7-C7-N2	-6.23	110.97	121.98
2	C	2	BDP	C1-C2-C3	5.33	117.41	109.64
3	D	4	BDP	O5-C5-C6	5.31	125.56	106.59
3	D	3	NAG	C8-C7-N2	5.13	124.63	116.12
3	D	3	NAG	O3-C3-C2	5.06	119.91	109.40
3	D	3	NAG	C1-O5-C5	5.00	118.88	112.19
3	D	4	BDP	C2-C3-C4	-4.56	102.85	110.86
3	D	4	BDP	C1-C2-C3	-4.21	103.52	109.64
3	D	2	BDP	C1-C2-C3	4.20	115.76	109.64
2	C	2	BDP	C3-C4-C5	3.68	115.63	109.30
3	D	3	NAG	C4-C3-C2	-3.43	105.99	111.02
2	C	3	NAG	C3-C4-C5	3.43	116.45	110.23
3	D	2	BDP	C3-C4-C5	3.40	115.15	109.30
3	D	4	BDP	O3-C3-C4	3.37	118.32	110.38
2	C	1	NAG	O5-C5-C4	-3.34	103.67	109.70
2	C	1	NAG	C1-C2-N2	-3.33	106.87	110.73
2	C	1	NAG	O5-C1-C2	-3.22	106.28	109.52
3	D	3	NAG	C1-C2-N2	-3.15	105.46	110.43
2	C	1	NAG	C1-O5-C5	3.15	119.74	113.65
3	D	4	BDP	O6A-C6-C5	-3.13	109.51	120.81
3	D	2	BDP	O4-C4-C3	3.12	117.73	110.38
3	D	4	BDP	O3-C3-C2	2.94	116.05	110.05
3	D	3	NAG	O5-C5-C6	2.89	113.29	107.66
3	D	4	BDP	O2-C2-C3	2.77	115.89	110.15
3	D	3	NAG	O7-C7-C8	-2.75	117.15	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O1-C1-C2	2.72	114.88	109.22
2	C	1	NAG	O4-C4-C5	-2.62	102.86	109.32
2	C	3	NAG	O3-C3-C4	2.58	116.47	110.38
3	D	3	NAG	O5-C1-C2	-2.47	107.47	111.29
3	D	2	BDP	O5-C1-C2	2.45	116.62	110.79
2	C	2	BDP	O5-C1-C2	2.41	116.54	110.79
2	C	1	NAG	C2-N2-C7	-2.39	117.51	123.11
2	C	1	NAG	C6-C5-C4	-2.39	107.16	113.02
2	C	3	NAG	C1-O5-C5	2.26	115.21	112.19
3	D	4	BDP	O6B-C6-C5	2.26	121.78	113.64
3	D	2	BDP	O2-C2-C3	2.22	114.75	110.15
3	D	3	NAG	O7-C7-N2	-2.17	118.14	121.98
3	D	4	BDP	O4-C4-C3	2.10	115.33	110.38
2	C	3	NAG	O5-C5-C6	2.01	111.58	107.66

There are no chirality outliers.

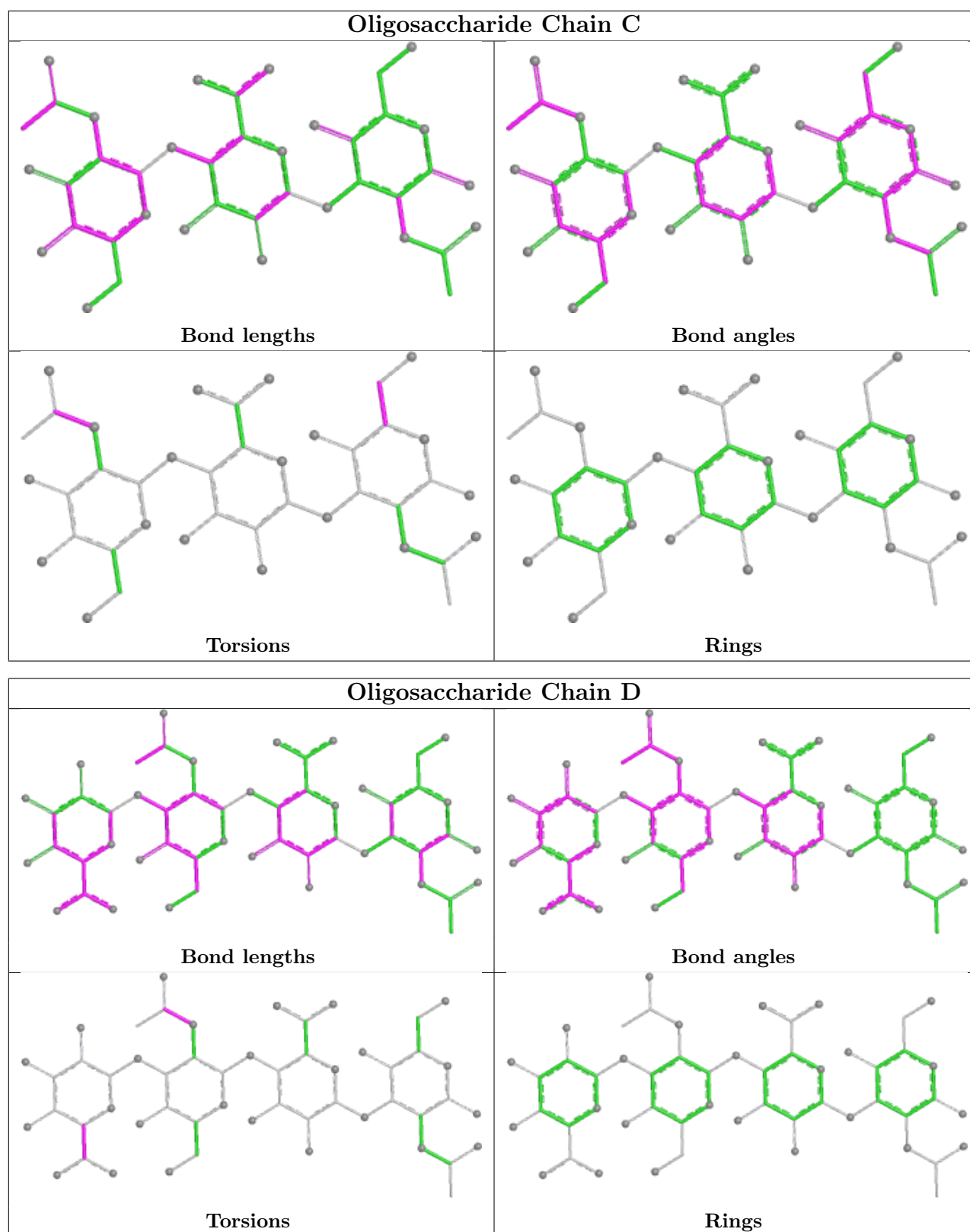
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	BDP	C4-C5-C6-O6A
3	D	4	BDP	C4-C5-C6-O6B
2	C	3	NAG	C8-C7-N2-C2
2	C	3	NAG	O7-C7-N2-C2
3	D	3	NAG	C8-C7-N2-C2
3	D	3	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	P4K	B	701	-	8,8,44	0.54	0	7,7,43	0.66	0
4	P4K	A	701	-	11,11,44	0.50	0	10,10,43	0.75	0
5	MES	A	702	-	12,12,12	0.98	0	15,16,16	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	P4K	B	701	-	-	0/6/6/42	-
4	P4K	A	701	-	-	4/9/9/42	-
5	MES	A	702	-	-	6/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

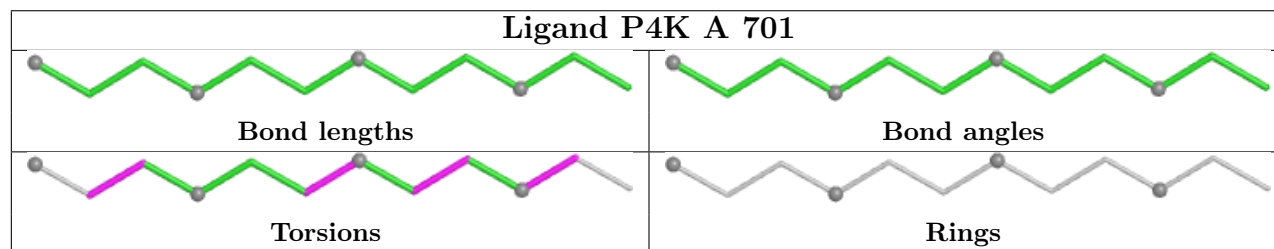
Mol	Chain	Res	Type	Atoms
5	A	702	MES	N4-C7-C8-S
5	A	702	MES	C7-C8-S-O3S
4	A	701	P4K	O8-C15-C16-O9
5	A	702	MES	C8-C7-N4-C3
5	A	702	MES	C8-C7-N4-C5
4	A	701	P4K	C14-C13-O7-C12
5	A	702	MES	C7-C8-S-O1S
5	A	702	MES	C7-C8-S-O2S
4	A	701	P4K	C9-C10-O6-C11
4	A	701	P4K	O6-C11-C12-O7

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	P4K	1	0
5	A	702	MES	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	618/644 (95%)	-0.32	5 (0%) 82 83	13, 30, 54, 74	3 (0%)
1	B	608/644 (94%)	0.04	12 (1%) 65 65	18, 38, 63, 96	2 (0%)
All	All	1226/1288 (95%)	-0.14	17 (1%) 73 73	13, 34, 60, 96	5 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	481	THR	4.2
1	B	469	THR	3.8
1	B	482	ILE	3.1
1	B	26	TYR	3.0
1	A	291	ALA	2.7
1	B	228	PHE	2.6
1	B	230	TRP	2.6
1	B	505[A]	GLU	2.5
1	B	61	ALA	2.4
1	B	403	ALA	2.3
1	A	288	GLY	2.3
1	B	235	ILE	2.3
1	B	468	GLY	2.3
1	A	532	ALA	2.2
1	A	560	VAL	2.1
1	A	502	TYR	2.1
1	B	62	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

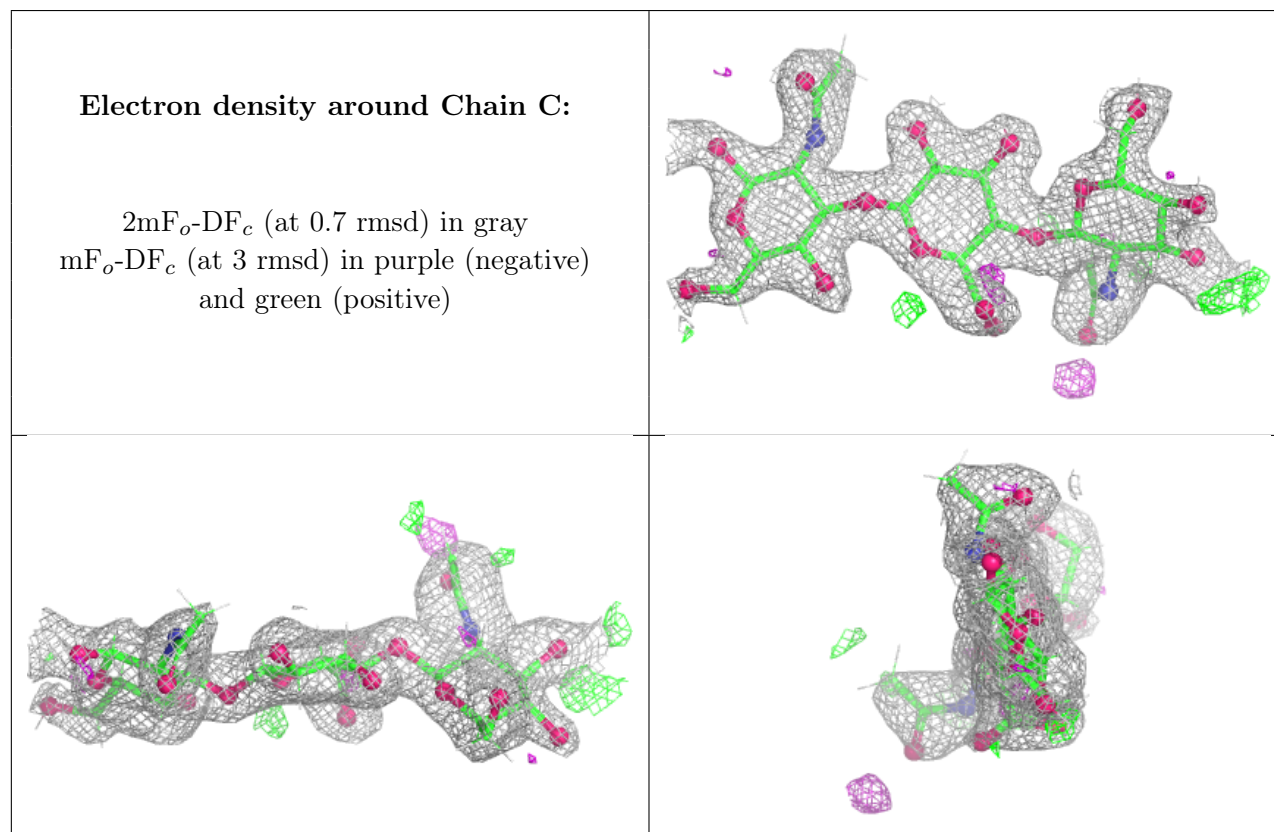
There are no non-standard protein/DNA/RNA residues in this entry.

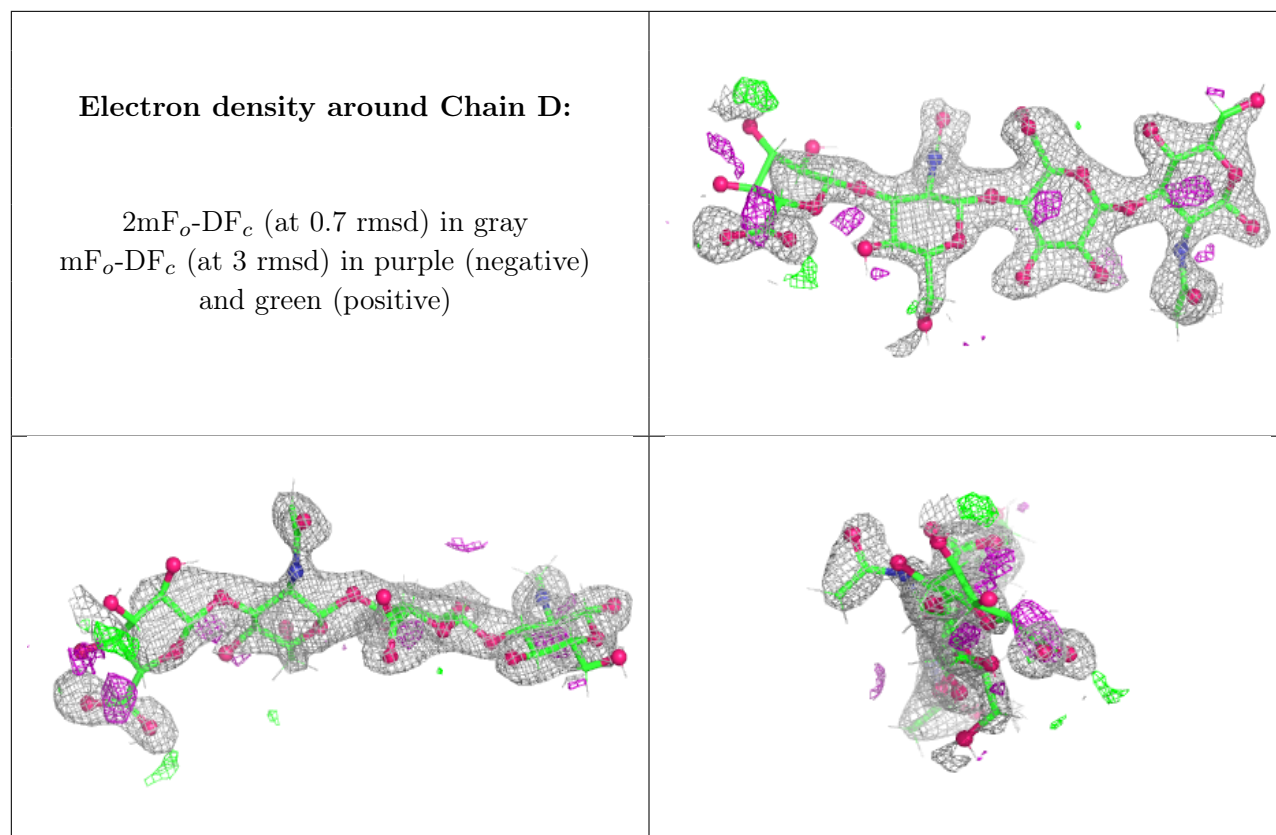
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BDP	D	4	12/13	0.64	0.18	30,78,93,97	2
3	NAG	D	3	14/15	0.71	0.16	30,64,70,72	2
2	NAG	C	3	14/15	0.78	0.14	30,49,58,75	2
3	BDP	D	2	12/13	0.85	0.11	30,51,60,67	2
3	NAG	D	1	15/15	0.89	0.10	30,58,66,67	2
2	NAG	C	1	15/15	0.89	0.10	30,41,49,59	2
2	BDP	C	2	12/13	0.93	0.08	27,36,51,59	2

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



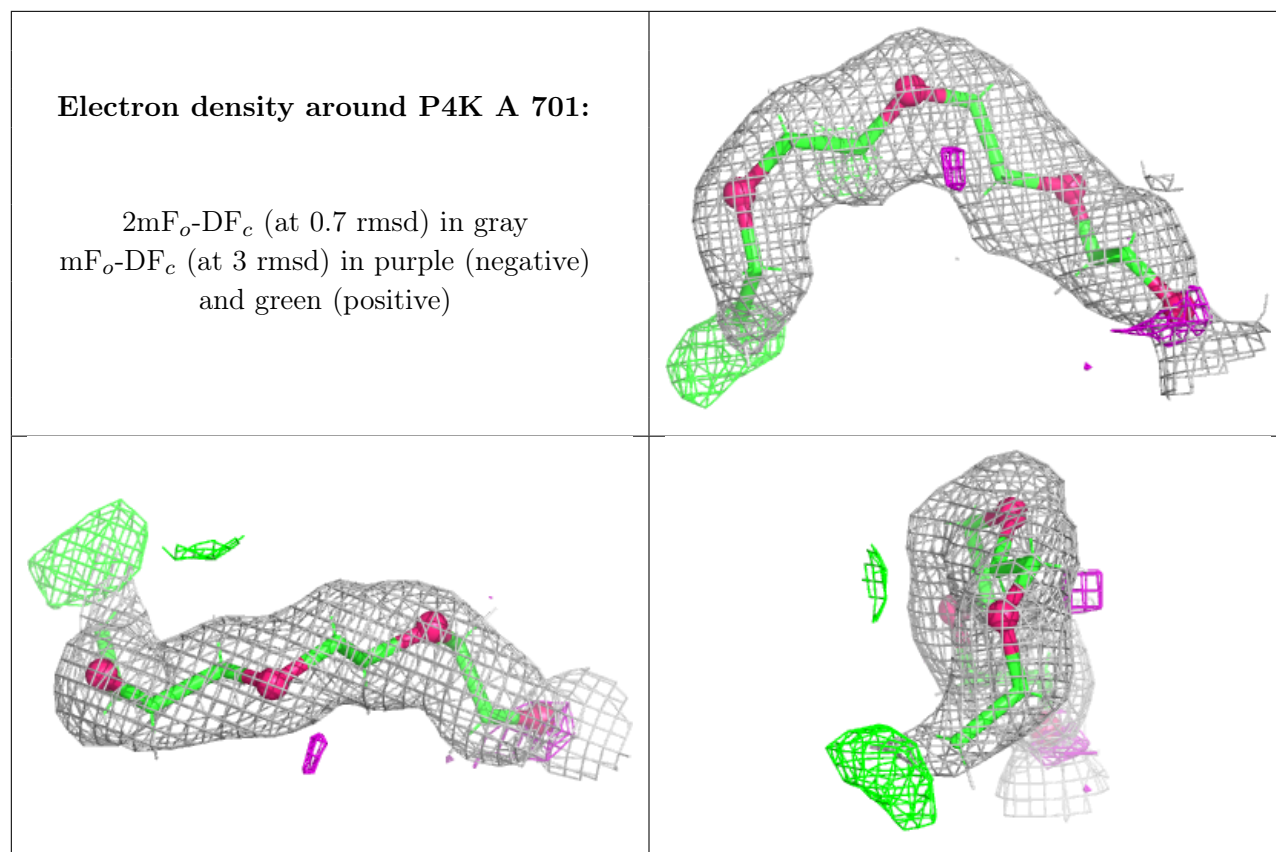


6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MES	A	702	12/12	0.66	0.17	48,60,132,136	0
4	P4K	A	701	12/45	0.88	0.11	27,34,45,47	1
4	P4K	B	701	9/45	0.89	0.11	30,45,48,50	1
6	ZN	B	702	1/1	0.99	0.03	35,35,35,35	0
6	ZN	A	703	1/1	1.00	0.02	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.